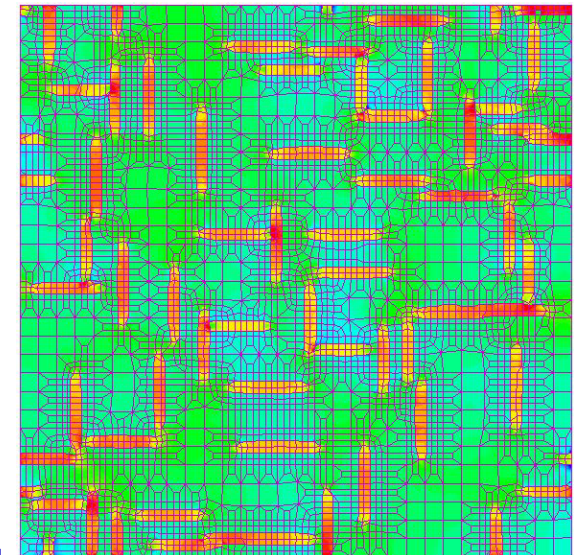
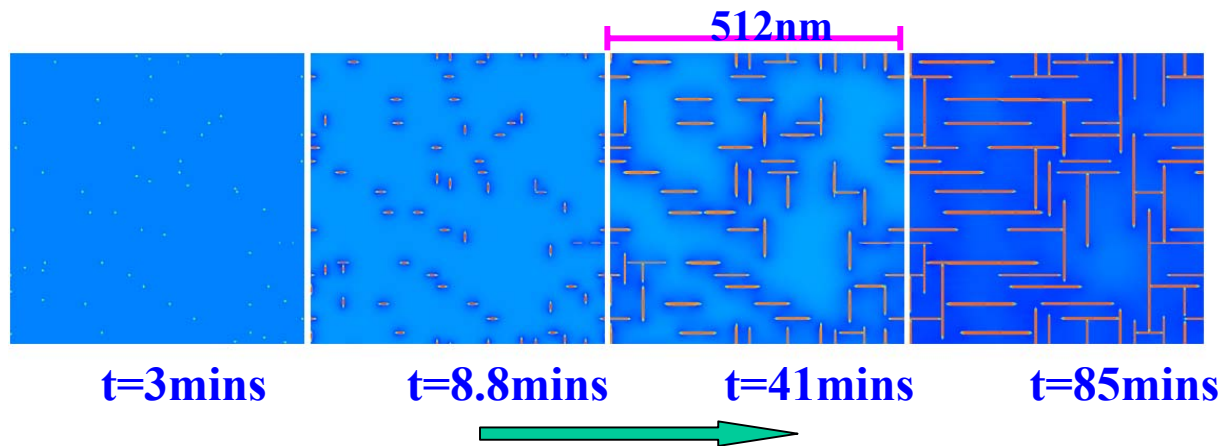
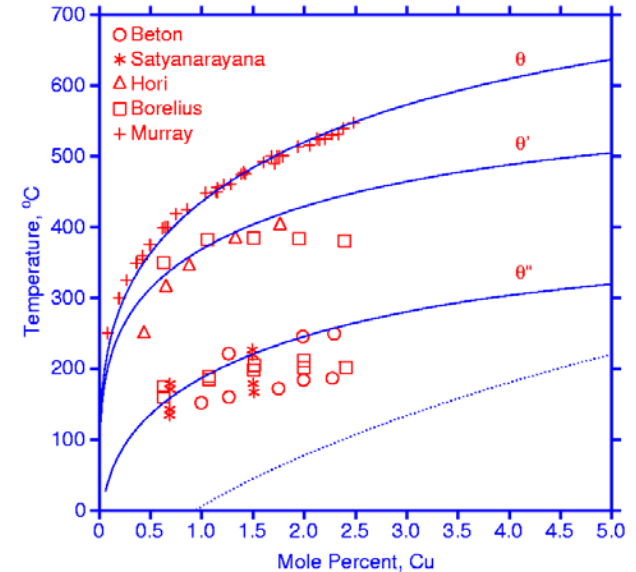


ITR: Computational Tools for Multicomponent Materials Design

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Stephen Langer (NIST), Christopher Wolverton (Ford). ITR-0205232

Phases	Source	ΔH (kJ/mol)	ΔS (J/mol/K)
Al_2Cu (θ)	Present Assessment	-16.0	-2.719
	First-Principles	-16.2 (Present)	-2.079
Al_2Cu (θ')	Present Assessment	-16.8	-5.434
	First-Principles	-20.5 (Present)	-5.155
Al_3Cu (θ'')	Present Assessment	-8.4	0.385
	First-Principles	-9.6 (Present)	0.565



First complete integration of first-principles calculations, database modeling (CALPHAD), phase-field simulation, and object-oriented finite element simulation (OOF) for θ' formation from fcc and its elastic response in Al-Cu alloys.

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There have been two PhD and two MS graduations supported by this project. This project currently support *five women graduate students*.

Current Postdoctoral Fellows

Edwin Garcia, Shenyang Hu, Chinnappan Ravi , Keita Teranishi, Yi Wang, Peng Yu, Wenxiang Zhu

Current Graduate Students

Maria Emelianenko, Weiming Feng, Qiu-Jiang Li, Manjeera Mantina, Dongwon Shin, Anusha Srirama, Tao Wang, Hui Zhang

Project Alumni

PhD: Chao Jiang, Keita Teranishi

MS: William Stevenson, Jianwei Wang

Postdoc: Shihuai Zhou, Jingzhi Zhu



People with
names in bold
are shown in the
photo.